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Table I. Some Common Methods of Computational Thermochemistry [a]

Method	*Applicability*		*Cost*			*Reliability*[b]	
	Type	*Size*	*Software*	*Computer*	*Personnel*	*Accuracy*[c]	*Precision*[d]
empirical (e.g., Benson groups)	common organic	any	$	¢	$	A-	B+
molecular mechanics (e.g., MM3)	common organic	100,000 atoms	$	¢¢¢	$$	A-	B
semiempirical MO theory (e.g., MNDO/d)	organic, some inorganic	500 atoms	$	$	$$	C+	C-
density functional theory (e.g., B3LYP)	all[e]	50 atoms[f]	$$$	$$	$$$	B-	C+
CBS-4 (MO theory)	all[e]	20 atoms[f]	$$$	$$$	$$$	B	B-
BAC-MP4 (corr. MO theory)	organic, some inorganic	20 atoms[f]	$$$	$$$	$$$$	B+	B
PCI-80 (corr. MO theory)	all[e]	20 atoms[f]	$$$	$$$	$$$$	B+	B-
G2 (MO theory)	all[e]	6 heavies[f]	$$$	$$$$	$$$	A-	B
CCSD(T) with basis set extrapolation (MO theory)	all[e]	3 heavies[f]	$$$	$$$$$$	$$$$	A	A-

[a] The opinions in this Table are those of the authors and do not necessarily represent those of the authors of other chapters in this book.
[b] DFT methods are more robust than MO methods for molecules that contain transition metals, although both are less accurate for transition-metal species than for organics.
[c] Typical performance for a large set of molecules (i.e., mean error).
[d] Worst-case performance among a large set of molecules (i.e., largest error).
[e] Subject to availability of basis sets.
[f] Light atoms add less than heavy atoms to the computational expense; “heavy” means lithium or heavier.